

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
 Data File : BF132588.D
 Acq On : 01 Mar 2023 13:32
 Operator : CG\JU
 Sample : 01701-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-13-GW01

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.240	446	451	463	rVB	1497381	1697244	3.40%	1.479%
2	5.634	510	518	521	rBV	3499801	3469381	6.95%	3.024%
3	6.622	682	686	691	rBV	2858260	2557063	5.12%	2.229%
4	7.004	747	751	757	rBV	1402930	1327510	2.66%	1.157%
5	7.569	842	847	850	rBV	4155011	4344136	8.70%	3.787%
6	7.957	854	913	915	rBV	5351954	49942925	100.00%	43.536%
7	8.286	966	969	972	rBV	2043157	1638856	3.28%	1.429%
8	8.463	994	999	1001	rVV2	695590	1240754	2.48%	1.082%
9	8.516	1001	1008	1010	rVV	1753316	3644108	7.30%	3.177%
10	8.551	1010	1014	1018	rVV3	2041587	3429675	6.87%	2.990%
11	8.633	1018	1028	1032	rVV4	1627281	3955175	7.92%	3.448%
12	8.745	1036	1047	1048	rVV	2497199	6330903	12.68%	5.519%
13	8.780	1051	1053	1054	rVV	1618443	1459284	2.92%	1.272%
14	8.804	1054	1057	1061	rVV	2477886	2540576	5.09%	2.215%
15	8.992	1086	1089	1097	rVB2	552890	639030	1.28%	0.557%
16	9.369	1148	1153	1156	rBV	7618318	7214881	14.45%	6.289%
17	10.051	1265	1269	1272	rBV	2187706	1845128	3.69%	1.608%
18	10.845	1399	1404	1407	rBV	5018269	4930614	9.87%	4.298%
19	11.545	1519	1523	1525	rBV	2214568	1926727	3.86%	1.680%
20	12.051	1605	1609	1614	rBV	610524	668901	1.34%	0.583%
21	13.139	1789	1794	1797	rBV	7363780	7441072	14.90%	6.486%
22	14.198	1970	1974	1977	rBV	1454502	1356387	2.72%	1.182%
23	15.751	2232	2238	2251	rVB	775365	1117193	2.24%	0.974%

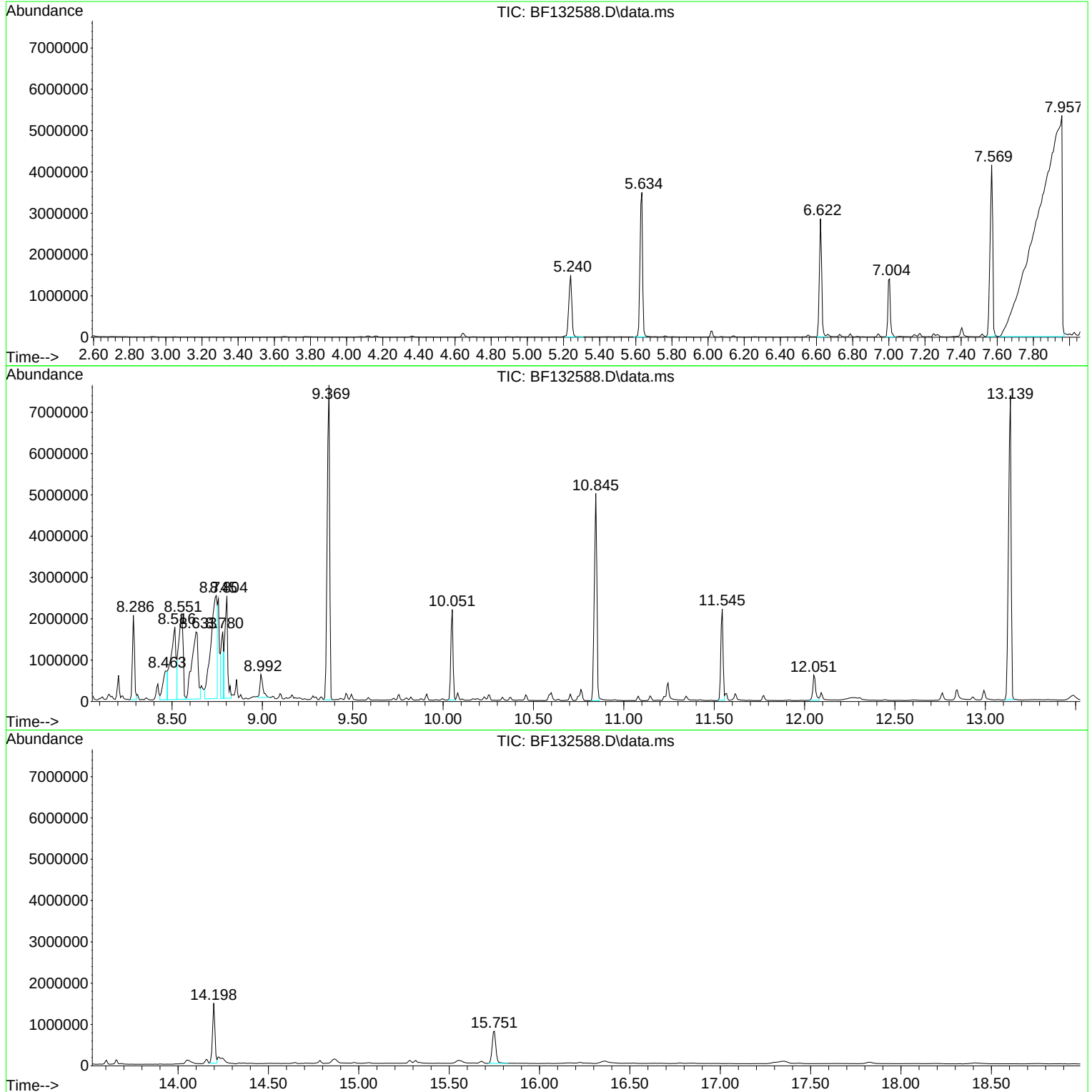
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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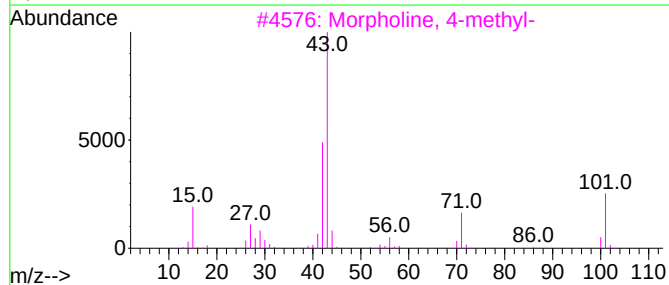
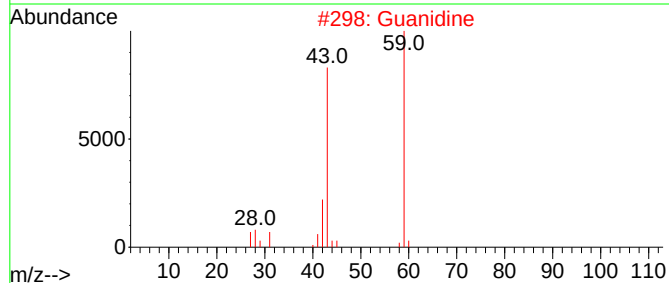
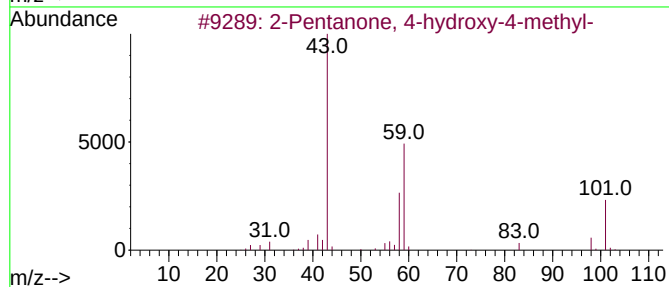
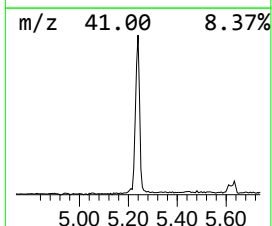
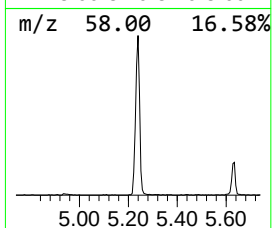
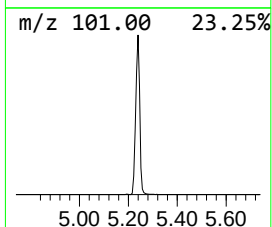
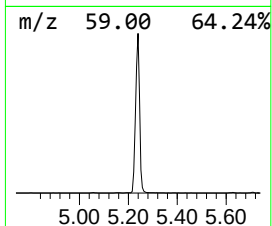
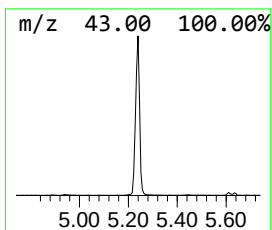
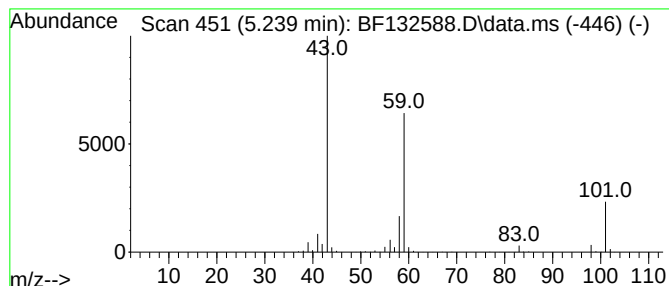
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.239	25.57 ng	1697240	1,4-Dichlorobenzene-d4	7.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Guanidine	59	CH5N3	000113-00-8	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Acetone	58	C3H6O	000067-64-1	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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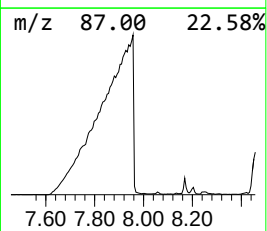
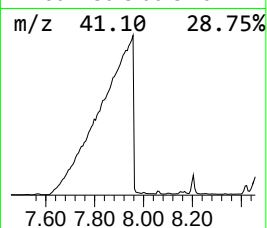
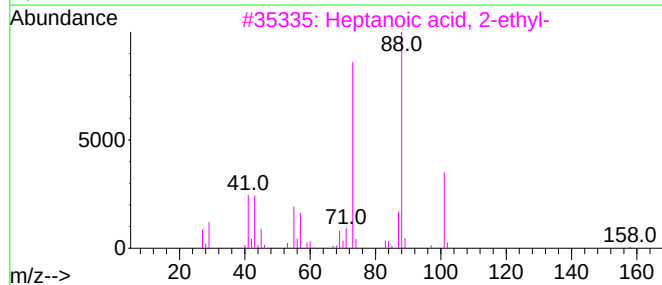
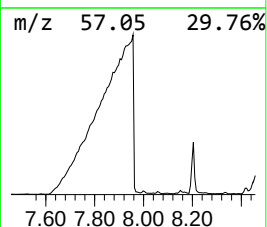
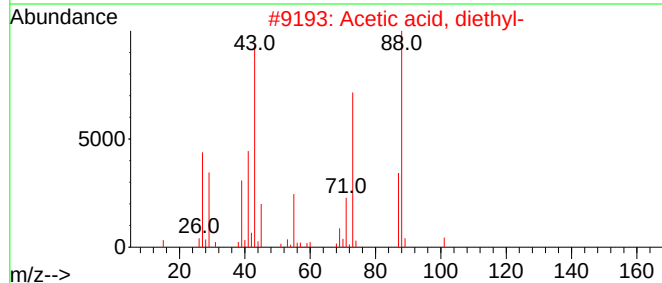
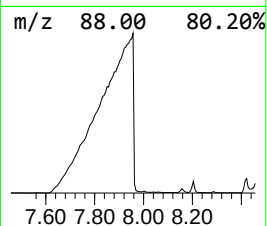
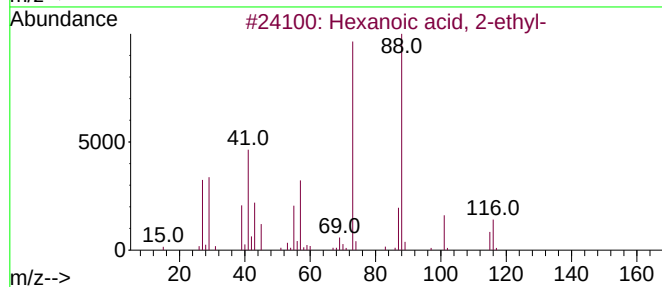
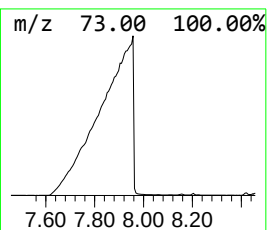
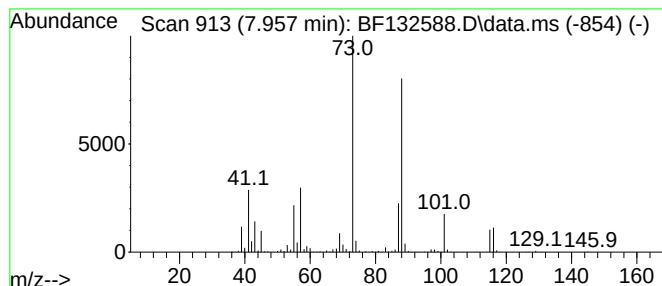
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	609.49 ng	49942900	Naphthalene-d8	8.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
3			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
4			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
5			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40



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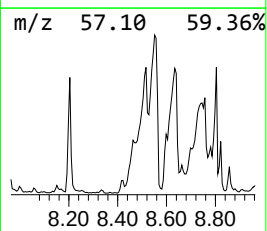
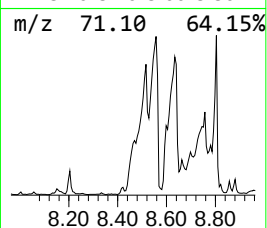
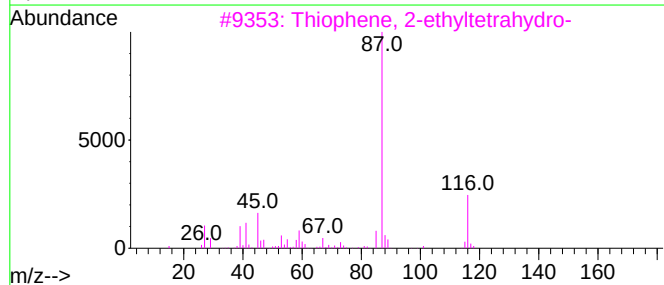
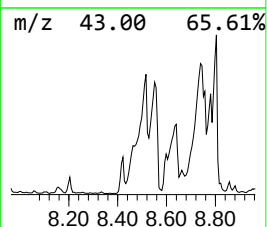
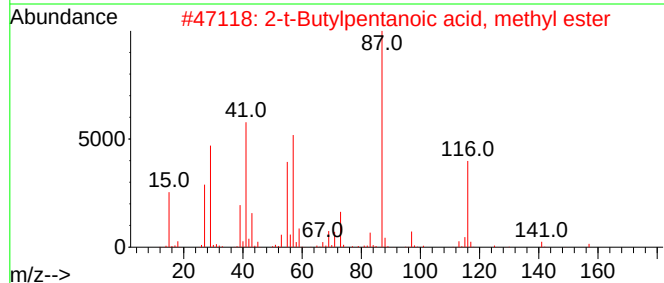
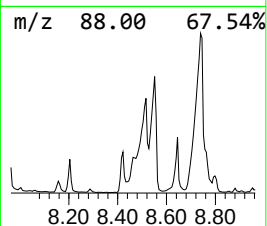
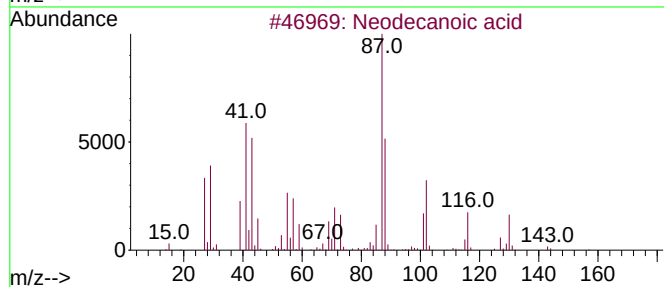
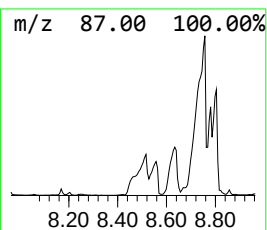
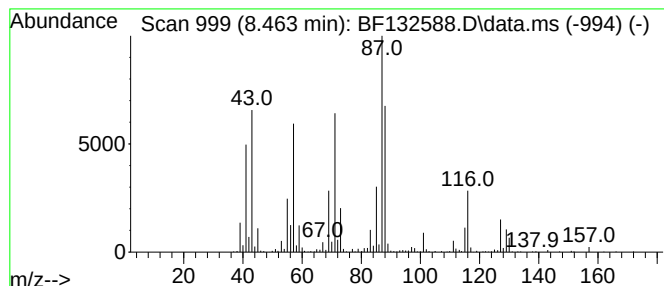
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Neodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	15.14 ng	1240750	Naphthalene-d8	8.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neodecanoic acid	172	C10H20O2	026896-20-8	53
2			2-t-Butylpentanoic acid, methyl ...	172	C10H20O2	1000202-22-5	38
3			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	35
4			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	22
5			2-[2-[2-[2-[2-[2-(2-Acetyloxy...	454	C20H38O11	1000351-90-6	22



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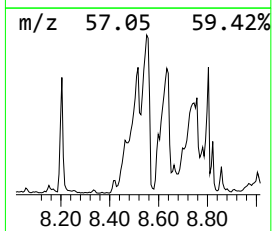
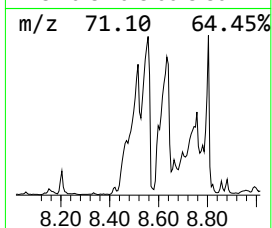
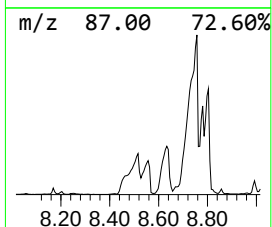
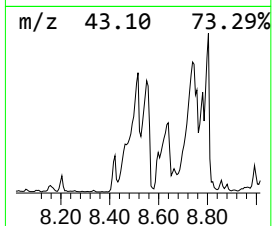
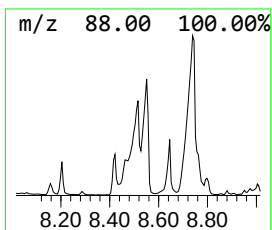
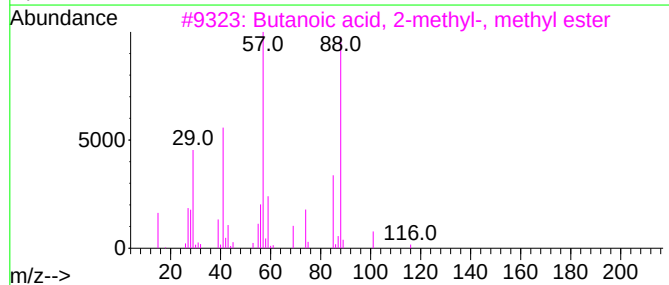
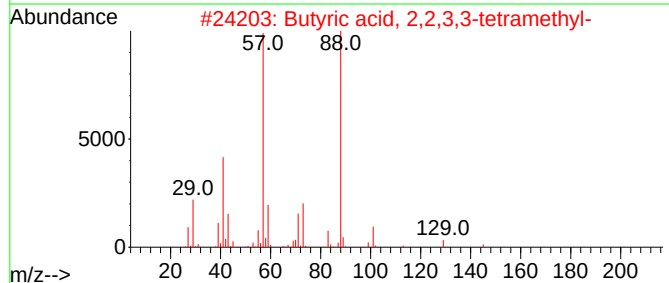
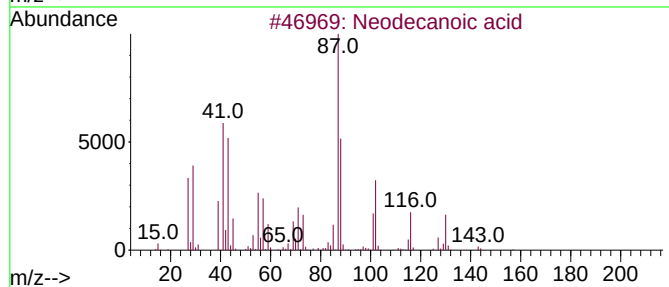
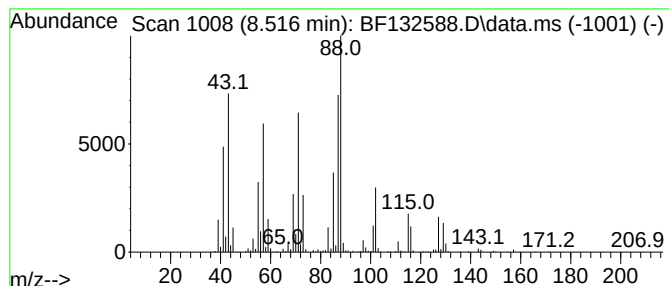
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Peak Number 4 unknown8.516 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.516	44.47 ng	3644110	Naphthalene-d8	8.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Neodecanoic acid	172	C10H20O2	026896-20-8	38
2		Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	35
3		Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	35
4		Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	27
5		Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	27



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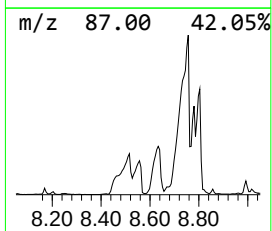
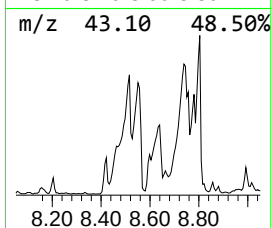
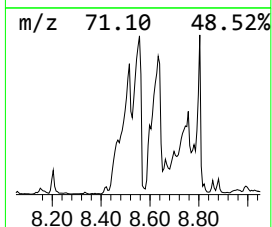
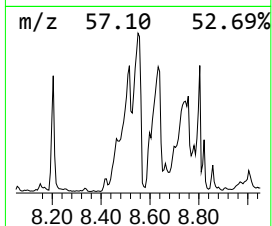
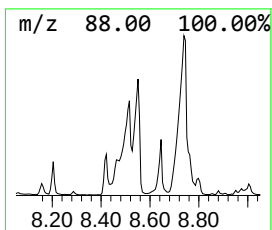
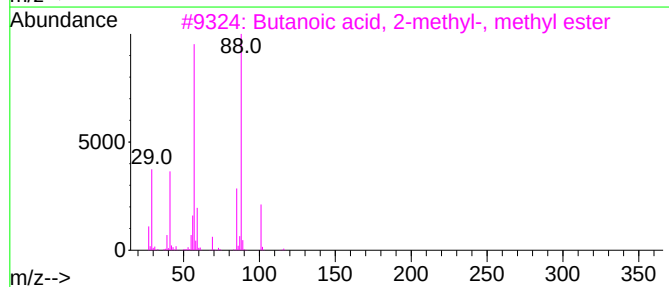
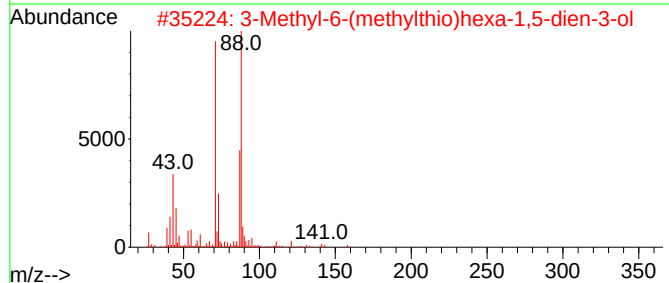
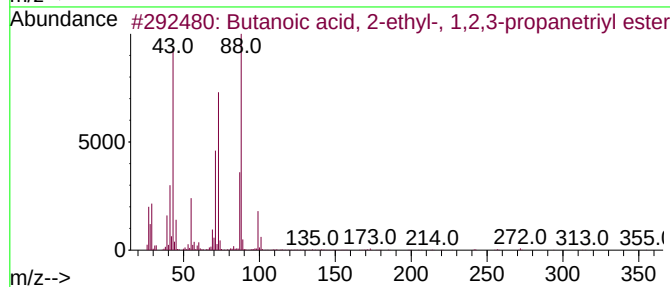
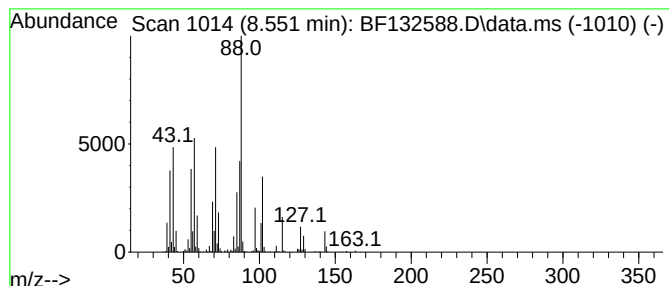
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butanoic acid, 2-ethyl-, 1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	41.85 ng	3429680	Naphthalene-d8	8.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
2			3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	40
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	35
4			Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	27
5			Butanoic acid, 2,3-dimethyl-, me...	130	C7H14O2	030540-29-5	25



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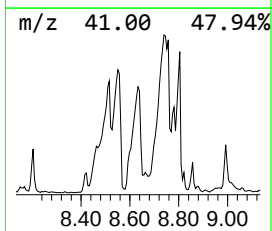
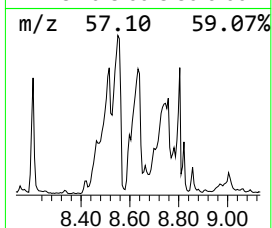
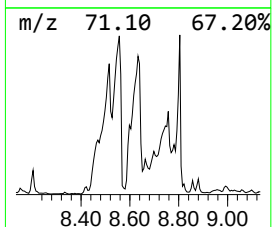
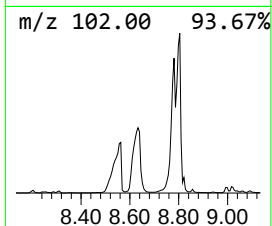
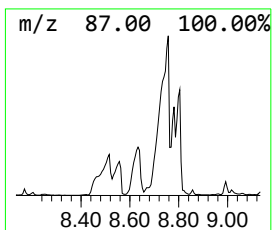
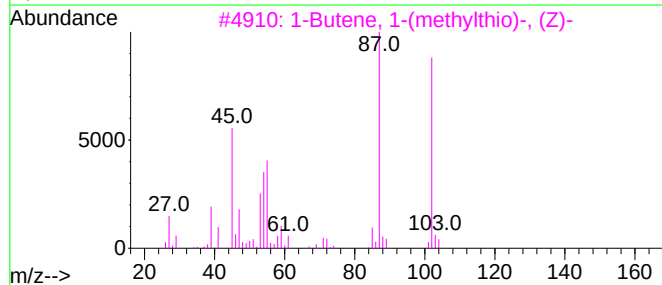
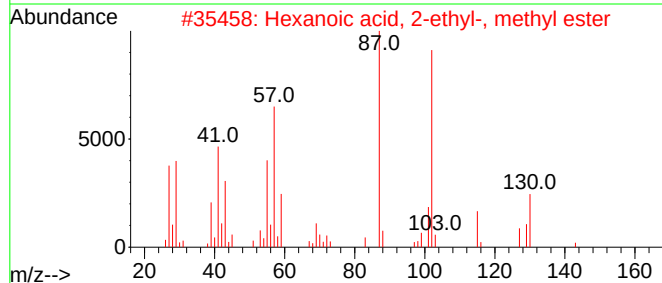
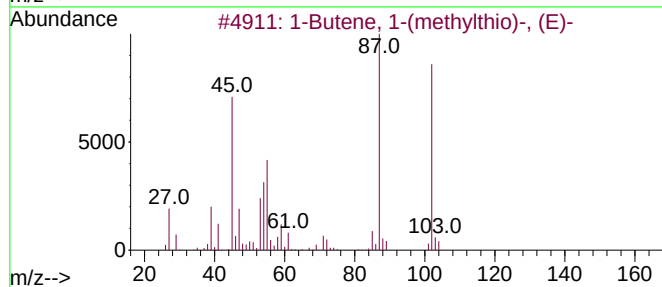
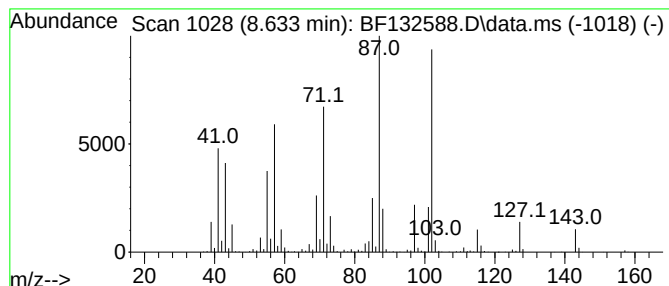
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown8.633 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.633	48.27 ng	3955180	Naphthalene-d8	8.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	43
2		Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	38
3		1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	37
4		Butanoic acid, 2,3-dimethyl-, et...	144	C8H16O2	054004-42-1	30
5		2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
Data File : BF132588.D
Acq On : 01 Mar 2023 13:32
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-13-GW01

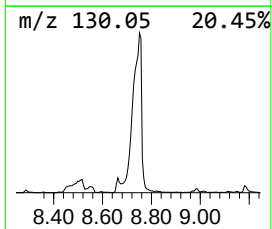
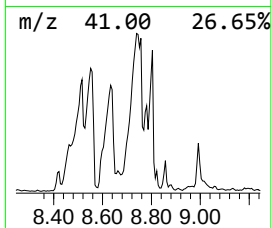
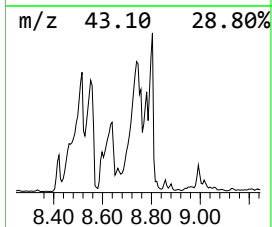
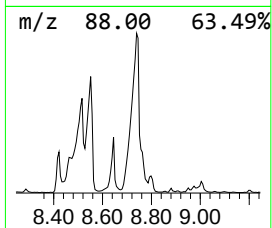
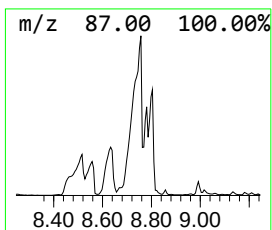
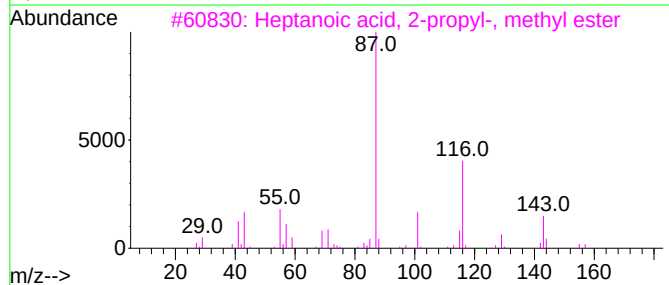
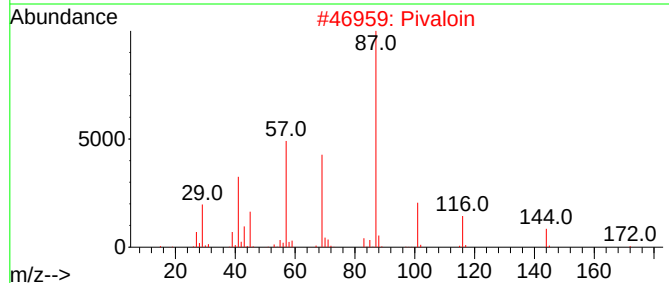
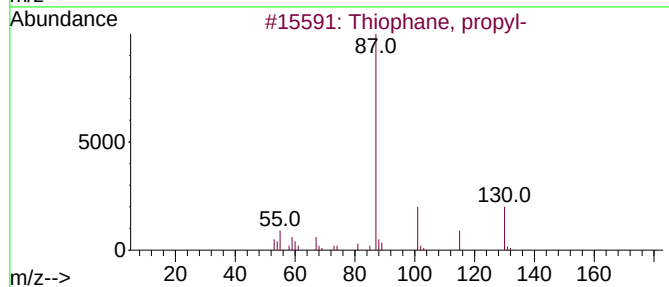
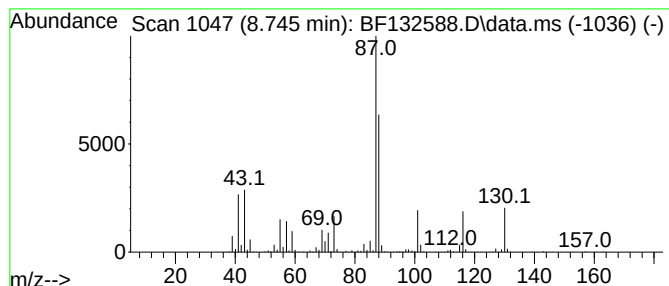
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Thiophane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.745	77.26 ng	6330900	Naphthalene-d8	8.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Thiophane, propyl-	130	C7H14S	001551-34-4	52
2		Pivaloin	172	C10H20O2	000815-66-7	47
3		Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	38
4		Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	37
5		Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
Data File : BF132588.D
Acq On : 01 Mar 2023 13:32
Operator : CG\JU
Sample : 01701-03
Misc :
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Instrument :
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ClientSampleId :
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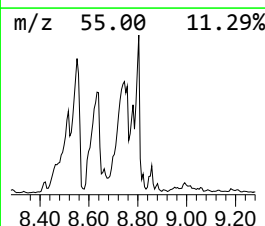
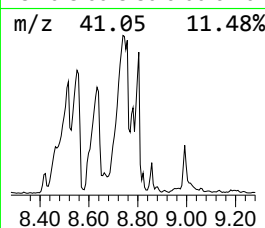
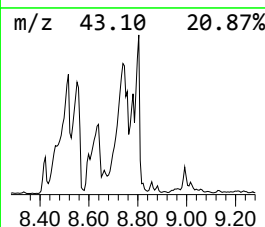
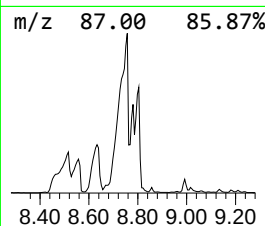
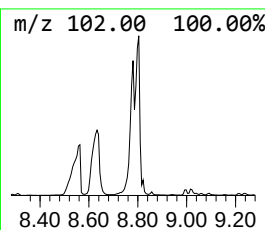
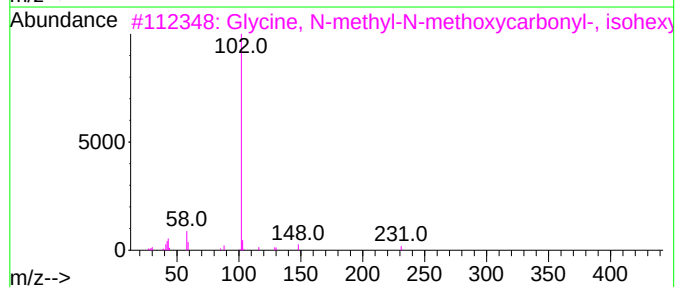
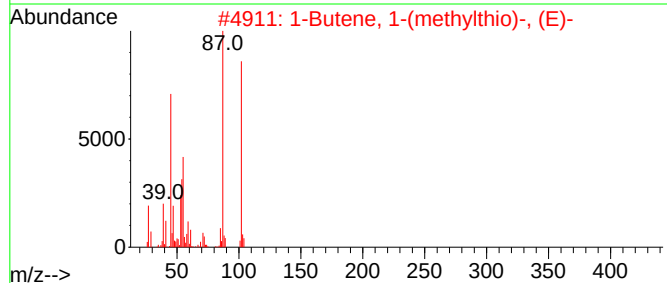
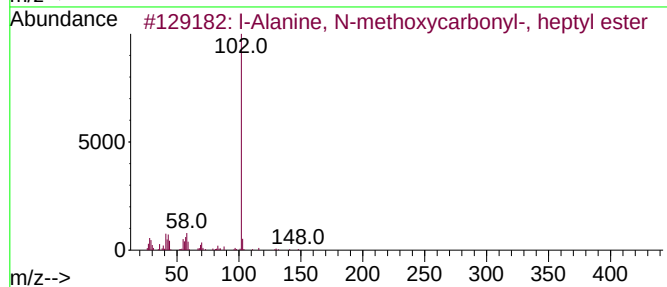
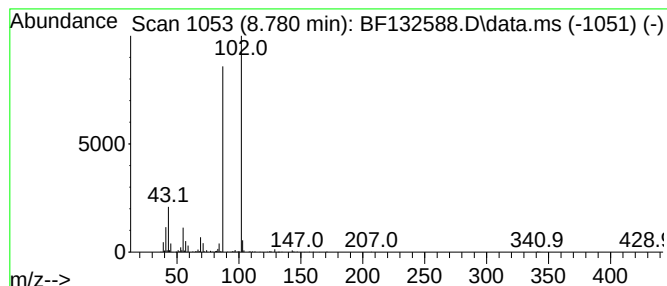
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown8.780 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.780	17.81 ng	1459280	Naphthalene-d8	8.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			l-Alanine, N-methoxycarbonyl-, h...	245	C12H23NO4	1000313-37-7	17
2			1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	9
3			Glycine, N-methyl-N-methoxycarbo...	231	C11H21NO4	1000320-60-6	9
4			Glycine, N-methyl-N-methoxycarbo...	301	C16H31NO4	1000320-61-2	9
5			l-Alanine, N-methoxycarbonyl-, d...	315	C17H33NO4	1000313-38-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
Data File : BF132588.D
Acq On : 01 Mar 2023 13:32
Operator : CG\JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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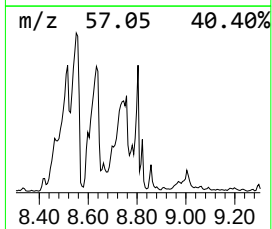
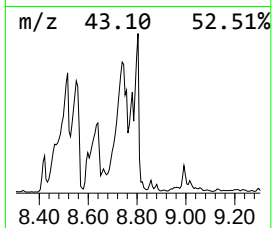
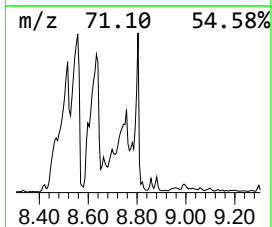
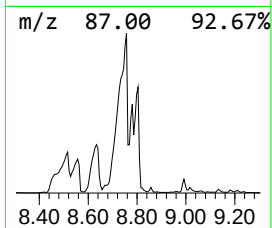
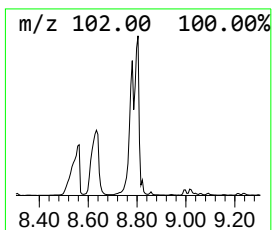
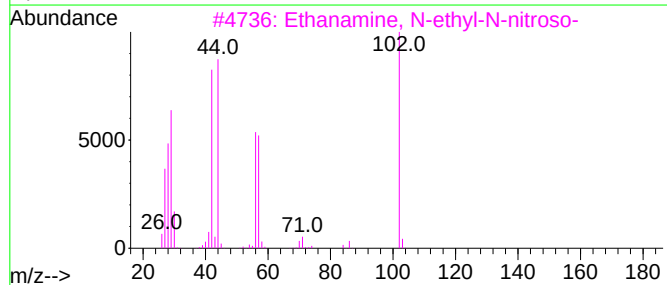
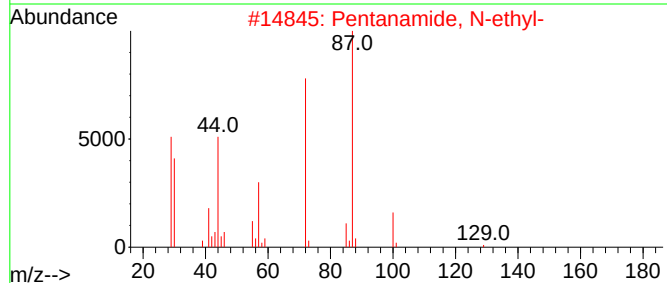
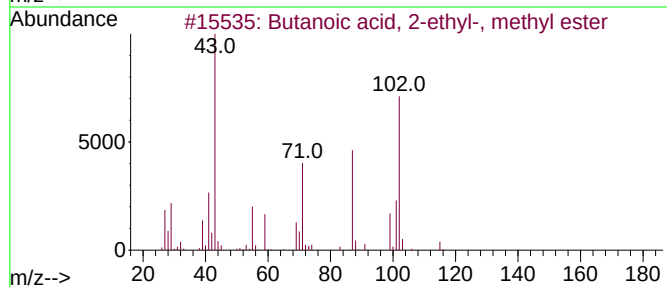
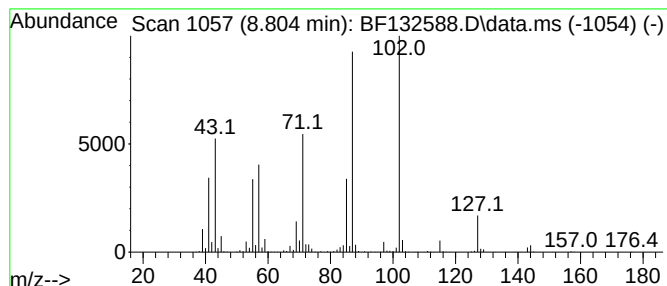
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Butanoic acid, 2-ethyl-, me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.804	31.00 ng	2540580	Naphthalene-d8	8.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	53
2			Pentanamide, N-ethyl-	129	C7H15NO	054007-33-9	25
3			Ethanamine, N-ethyl-N-nitroso-	102	C4H10N2O	000055-18-5	22
4			2-[2-[2-[2-(2-Acetyloxyethoxy...	366	C16H30O9	024997-24-8	14
5			2-t-Butylpentanoic acid, methyl ...	172	C10H20O2	1000202-22-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
Data File : BF132588.D
Acq On : 01 Mar 2023 13:32
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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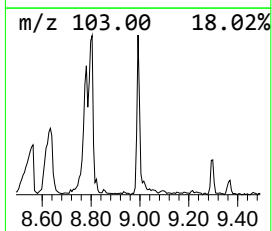
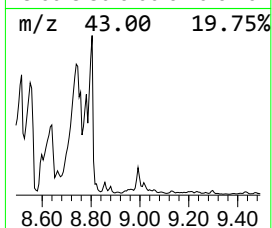
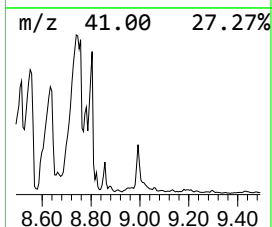
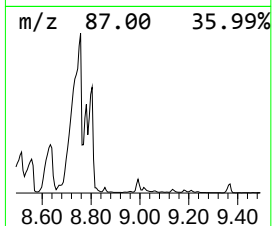
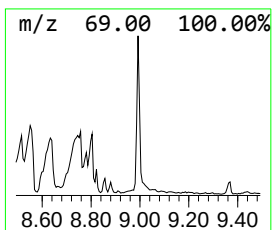
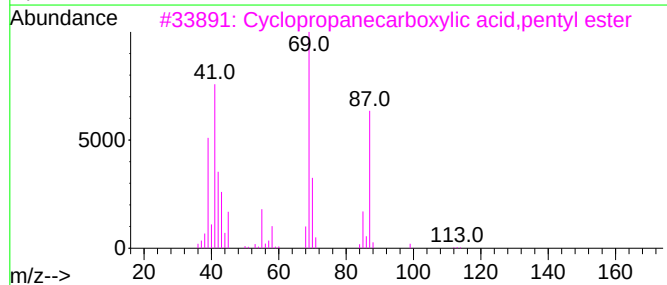
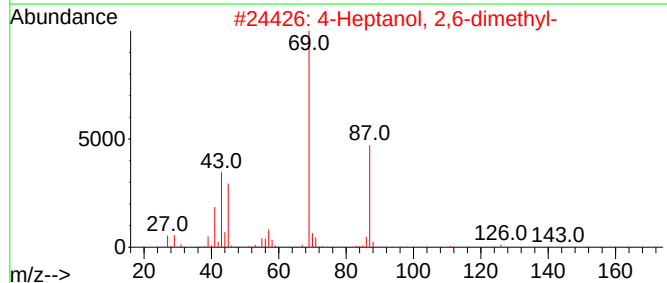
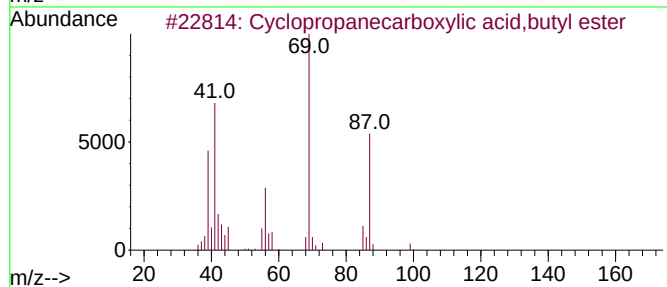
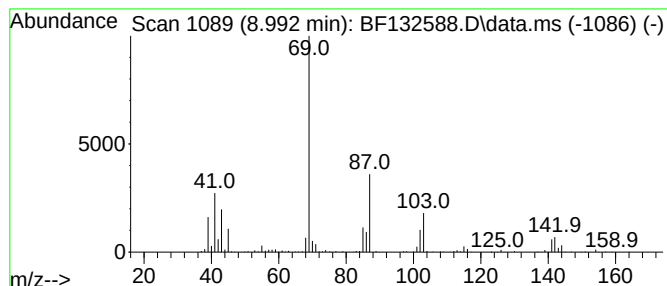
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Cyclopropanecarboxylic acid... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.992	7.80 ng	639030	Naphthalene-d8	8.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	59
2		4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	53
3		Cyclopropanecarboxylic acid, pent...	156	C9H16O2	060128-02-1	45
4		1,2-Hexanediol	118	C6H14O2	006920-22-5	42
5		2-Hydroxyethyl methacrylate	130	C6H10O3	000868-77-9	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
Data File : BF132588.D
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Sample : 01701-03
Misc :
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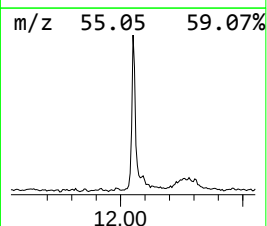
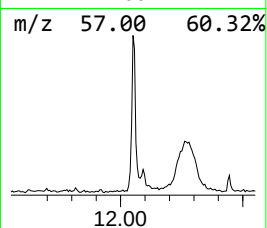
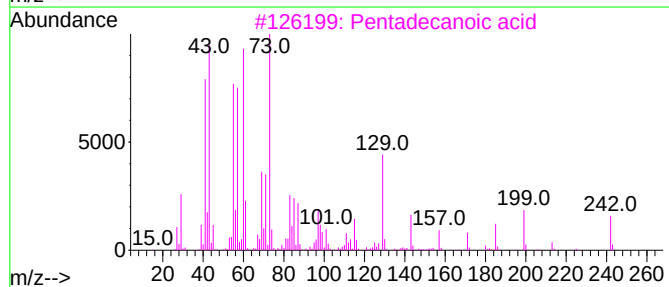
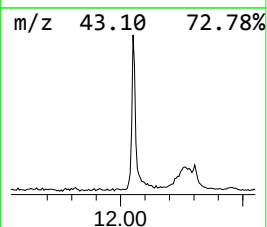
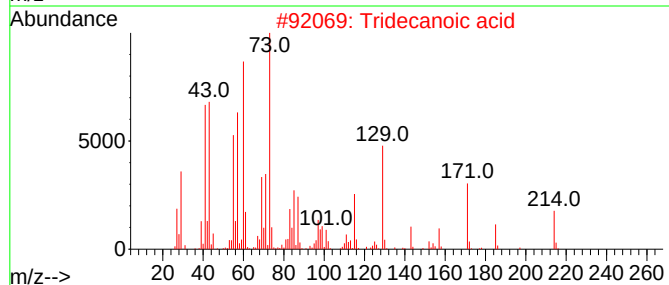
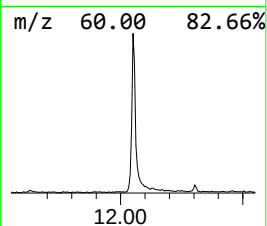
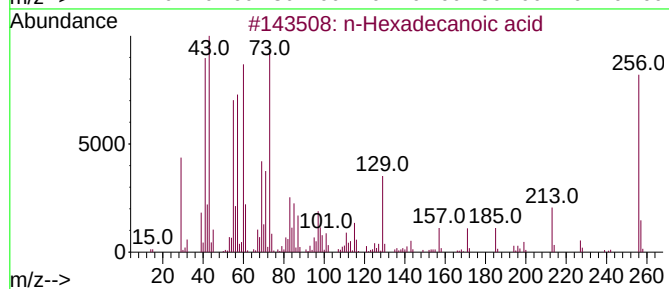
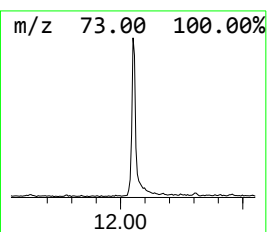
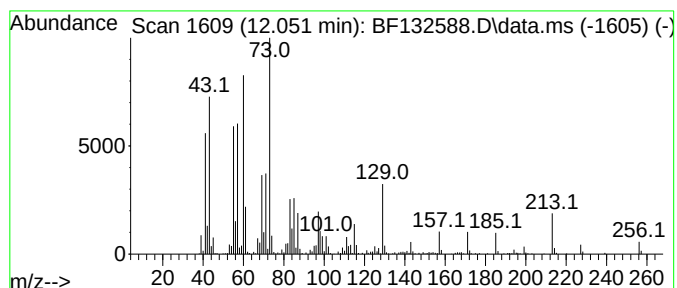
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.051	6.94 ng	668901	Phenanthrene-d10	11.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
Data File : BF132588.D
Acq On : 01 Mar 2023 13:32
Operator : CG\JU
Sample : 01701-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Hexanoic acid, ...	7.957	609.5	ng	49942900	2	8.286	1638860	20.0
Neodecanoic acid	8.463	15.1	ng	1240750	2	8.286	1638860	20.0
unknown8.516	8.516	44.5	ng	3644110	2	8.286	1638860	20.0
Butanoic acid, ...	8.551	41.9	ng	3429680	2	8.286	1638860	20.0
unknown8.633	8.633	48.3	ng	3955180	2	8.286	1638860	20.0
Thiophane, propyl-	8.745	77.3	ng	6330900	2	8.286	1638860	20.0
unknown8.780	8.780	17.8	ng	1459280	2	8.286	1638860	20.0
Butanoic acid, ...	8.804	31.0	ng	2540580	2	8.286	1638860	20.0
Cyclopropanecar...	8.992	7.8	ng	639030	2	8.286	1638860	20.0
n-Hexadecanoic ...	12.051	6.9	ng	668901	4	11.545	1926730	20.0